Density functional calculation of the 2D potential surface and deuterium isotope effect on ^{13}C chemical shifts in picolinic acid *N*-oxide. Comparison with experiment.

Autorzy

J. Stare

Aneta Jezierska

G. Ambrožič

I. J. Košir

J. Kidrič

Aleksander Koll

J. Mavri

D. Hadži

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2D free energy surfaces $V = V(r_{OH}, r_{O\cdots O})$ for the intramolecular H-bond in the title compound were calculated by the DFT method and used in the calculation of primary and secondary chemical shifts of the compound dissolved in chloroform and acetonitrile. Solvent effects were accounted for by the SCRF/PCM method. The corresponding two-dimensional chemical shift surfaces with included solvent reaction field were obtained using the Continuous Set of Gauge Transformations approach at the B3LYP/6-311+G(2d,2p) level of theory. The chemical shifts were estimated as quantum averages along the two internal coordinates in the hydrogen bond and along several vibrational levels according to the Boltzmann distribution at room temperature. Fairly good agreement between the experimental and calculated isotope effects was obtained. 1D and 2D NMR spectra of solutions of picolinic acid N-oxide and its deuterated analogue were recorded and assigned.

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